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**SYNTHESIS AND CHARACTERIZATION OF AN ORGANTHALLIUM-
PHOSPHORUS ADDUCT: CRYSTAL STRUCTURE OF $(\text{Me}_3\text{SiCH}_2)_3\text{Tl}\cdot\text{P}(\text{SiMe}_3)_3$**

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Abstract

The organothallium phosphorus adduct $(\text{Me}_3\text{SiCH}_2)_3\text{Tl}\cdot\text{P}(\text{SiMe}_3)_3$ (**1**) was prepared by combining $(\text{Me}_3\text{SiCH}_2)_3\text{Tl}$ and $\text{P}(\text{SiMe}_3)_3$ at room temperature. Compound **1** was characterized by ^1H , $^{13}\text{C}\{^1\text{H}\}$, and $^{31}\text{P}\{^1\text{H}\}$ NMR, partial elemental analysis, EI mass spectrometry, and single-crystal X-ray analysis, the first to be reported for a thallium-group 15 adduct. Crystal data for **1**: trigonal system, space group $P\bar{3}_1$, with $a = 16.063(6)$ Å, $c = 12.148(3)$ Å, $D_{\text{calcd}} = 1.315$ g cm $^{-3}$, and $V = 2714.3(11)$ Å 3 for $Z = 3$. Refinement converged at $R = 0.042$ ($R_w = 0.045$). The Tl-P bond length in **1**, previously unreported for compounds of this type, was found to be 2.922(3) Å.

INTRODUCTION

As a result of our efforts to find facile methods of forming 13-15 bonds, we have prepared and characterized a variety of new and interesting compounds¹. Among these are Lewis acid-base

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adducts of the type $R_3M \cdot E(SiMe_3)_3$ ($R = Me_3SiCH_2$, $M = Ga$, $E = As$ or P ; ^{1c} $M = In$, $E = As$ ^{1a} or P ^{1c}; $R = Ph$ ^{1a,b}, $M = Ga$, $E = As$ or P). The successful isolation of these compounds motivated us to continue our studies of 13-15 adducts, specifically those containing thallium. Although thallium-group 15 adducts have been prepared², no solid-state structures of such compounds have been reported.

To this end, herein, we report the synthesis and structural characterization of the novel organothallium phosphorus compound $(Me_3SiCH_2)_3Tl \cdot P(SiMe_3)_3$ (**1**).

EXPERIMENTAL

Synthesis

General Considerations. All manipulations of air- and moisture-sensitive materials were performed in a Vacuum Atmospheres HE-493 Dri-Lab containing an argon atmosphere or by general Schlenk techniques. Pentane and hexane were distilled over sodium-potassium alloy under dry dinitrogen. $(Me_3SiCH_2)_3Tl$ ³, and $P(SiMe_3)_3$ ⁴ were synthesized by literature procedures. ¹H, ¹³C{¹H}, and ³¹P{¹H} NMR spectra were recorded on a Varian Unity 400 spectrometer operating at 400, 100.6, and 161.9 MHz, respectively. ¹H and ¹³C{¹H} spectra were referenced to TMS by using the residual protons or carbons of deuterated benzene at δ 7.15 or 128 ppm, respectively. ³¹P{¹H} spectra were referenced externally to 85% H₃PO₄ at δ 0.00 ppm. All NMR samples were prepared in 5-mm tubes which were septum-sealed under argon. Melting points (uncorrected) were obtained with a Thomas-Hoover Uni-melt apparatus and capillaries were flame-sealed under argon. Elemental Analyses were performed by E+R Microanalytical Laboratory, Inc., Corona, NY. Mass spectral data were collected on a JEOL JMS-SX 102A spectrometer operating in the electron ionization mode at 20 eV. X-ray crystallographic data were obtained at -120 °C on a Rigaku AFC6/S diffractometer utilizing graphite-monochromated Mo-K α ($\lambda = 0.71073$ Å) radiation.

Preparation of $(\text{Me}_3\text{SiCH}_2)_3\text{Tl}\cdot\text{P}(\text{SiMe}_3)_3$ (**1**)

$(\text{Me}_3\text{SiCH}_2)_3\text{Tl}$ (0.466 g, 1.00 mmol) dissolved in 25 mL of pentane was added to a 250 mL round-bottomed screw-top flask equipped with a Teflon valve and magnetic stirbar. $\text{P}(\text{SiMe}_3)_3$ (0.251 g, 1.00 mmol) dissolved in 25 mL of pentane was added dropwise to the stirred $(\text{Me}_3\text{SiCH}_2)_3\text{Tl}$ solution. The resulting clear solution was stirred at room temperature outside of the dry box for 24 h. The volatiles were removed *in vacuo* to yield a faint-purple crystalline solid which was extracted into 5 mL of warm hexane. Cooling of the extract to $-30\text{ }^\circ\text{C}$ for 2 d afforded colorless X-ray quality crystals of **1** (0.562 g, 78.4%). mp. $68\text{--}71\text{ }^\circ\text{C}$. Anal. Calcd. (found) for $\text{C}_{21}\text{H}_{60}\text{PSi}_6\text{Tl}$: C, 35.20 (35.09); H, 8.44 (8.20). ^1H NMR (C_6D_6): δ 0.08, 0.90 [d, $-\text{CH}_2$, $^2J_{\text{Tl-H}} = 329\text{ Hz}$], 0.13 [d, $-\text{SiMe}_3$, $^4J_{\text{Tl-H}} = 7\text{ Hz}$], 0.33 [d, P-SiMe_3 , $^3J_{\text{P-H}} = 5\text{ Hz}$]. $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6): δ 2.07, 3.01 [d, $-\text{CH}_2\text{Si}(\underline{\text{CH}}_3)_3$, $^3J_{\text{Tl-C}} = 95\text{ Hz}$], 4.13 [d, $-\text{PSi}(\underline{\text{CH}}_3)_3$, $^2J_{\text{P-C}} = 12\text{ Hz}$], 29.02, 37.32 [d, $-\underline{\text{CH}}_2\text{Si}(\text{CH}_3)_3$, $^1J_{\text{Tl-C}} = 835\text{ Hz}$]. $^{31}\text{P}\{^1\text{H}\}$ NMR (C_6D_6): δ -251.7 (s). Mass spec.: m/z 451, $(\text{C}_{11}\text{H}_{33}\text{Si}_3\text{Tl})^+$; 379, $(\text{C}_8\text{H}_{22}\text{Si}_2\text{Tl})^+$; 250, $(\text{C}_9\text{H}_{27}\text{PSi})^+$.

X-Ray Crystal Structure Determination

Crystallographic data for **1** are summarized in Table 1. The crystal used was a colorless block which was mounted on a glass fiber with a viscous oil under a stream of cold dinitrogen. X-ray intensity data were recorded at $-120\text{ }^\circ\text{C}$ and the structures were solved by direct methods. Full-matrix least-squares refinement with weights based upon counter statistics was performed. Hydrogen atoms were incorporated at their calculated positions using a riding model in the later iterations of refinement which converged at $R = 0.042$ ($R_w = 0.045$). A final difference-Fourier synthesis revealed no unusual features (max. 1.64 , min. $-1.24\text{ e } \text{\AA}^{-3}$). Crystallographic calculations were performed using the NRCVAX⁵ suite of structure determination programs. For all structure-factor calculations, neutral atom scattering factors and their anomalous dispersion corrections were taken from ref. 6. Interatomic distances and angles are given in Table 2. Non-hydrogen atom fractional atomic coordinates are listed in Table 3. An ORTEP⁷

diagram showing the solid-state conformation and atom numbering scheme of **1** is presented in the Figure.

RESULTS AND DISCUSSION

The 1:1 mole ratio reaction of $(\text{Me}_3\text{SiCH}_2)_3\text{Tl}$ with $\text{P}(\text{SiMe}_3)_3$ at room temperature affords the adduct $(\text{Me}_3\text{SiCH}_2)_3\text{Tl}\cdot\text{P}(\text{SiMe}_3)_3$ (**1**) in a good yield. Compound **1** is a crystalline material which is stable over long periods of time under inert atmosphere. In addition, **1** is surprisingly stable upon exposure to air and moisture and does not decompose rapidly. Interestingly, the resonances observed in the ^1H , $^{13}\text{C}\{^1\text{H}\}$, and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of **1** have chemical shifts that are very close to those observed for the starting materials, which suggests that **1** dissociates in benzene solution at room temperature. The ^1H and $^{13}\text{C}\{^1\text{H}\}$ spectra also evidence the fact that the thallium atom, with its spin of 1/2, couples to the protons and carbon atoms of its three Me_3SiCH_2 - ligands (see references 2a and 2b for representative ^1H and ^{13}C spectral parameters of organothallium compounds).

Compound **1** crystallizes in the trigonal system with three molecules occupying the general positions of the $\text{P}3_1$ space group. In the solid state, this molecule adopts the conformation depicted in the Figure. The most noteworthy structural feature of **1** is the novel Tl-P bond length of 2.922(3) Å. This bond is longer than the sum of the covalent radii⁸ (2.62 Å) for the thallium and phosphorus atoms, which is not surprising due to the dative nature of the bond. The coordination geometry about the thallium center is that of a distorted tetrahedron with a mean C-Tl-C angle of 118.0° and a mean C-Tl-P angle of 98.1°. Mean bond angles at the P atom [$\text{Tl-P-Si} = 112.5^\circ > \text{Si-P-Si} = 106.3^\circ$] reflect the relayed effect of the steric compressions resulting from the angular deformations around Tl. Since Tl-P analogs of **1** are not known, comparison of its bond lengths and bond angles with similar compounds is confined to the analogous gallium and indium compounds $(\text{Me}_3\text{SiCH}_2)_3\text{Ga}\cdot\text{P}(\text{SiMe}_3)_3$ (**2**)^{1c} and $(\text{Me}_3\text{SiCH}_2)_3\text{In}\cdot\text{P}(\text{SiMe}_3)_3$ (**3**)^{1c}. As expected, the metal-phosphorus bond lengths of 2.646(3) and 2.771(2) Å in **2** and **3**, respectively, are significantly shorter than the observed thallium-

phosphorus linkage in **1**. Surprisingly, the observed degree of angular distortion around the thallium center in **1** is in accord with that seen in **2** [mean C-Ga-C angle = 116.7°, mean C-Ga-P angle = 100.3°] and **3** [mean C-In-C angle = 116.2°, mean C-In-P angle = 101.4°] despite the metal size difference.

Future investigations in this area will focus on determining the utility of **1** as a single-source precursor to TlP and on preparing alternate organothallium pnictogen compounds.

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SUPPLEMENTARY DATA

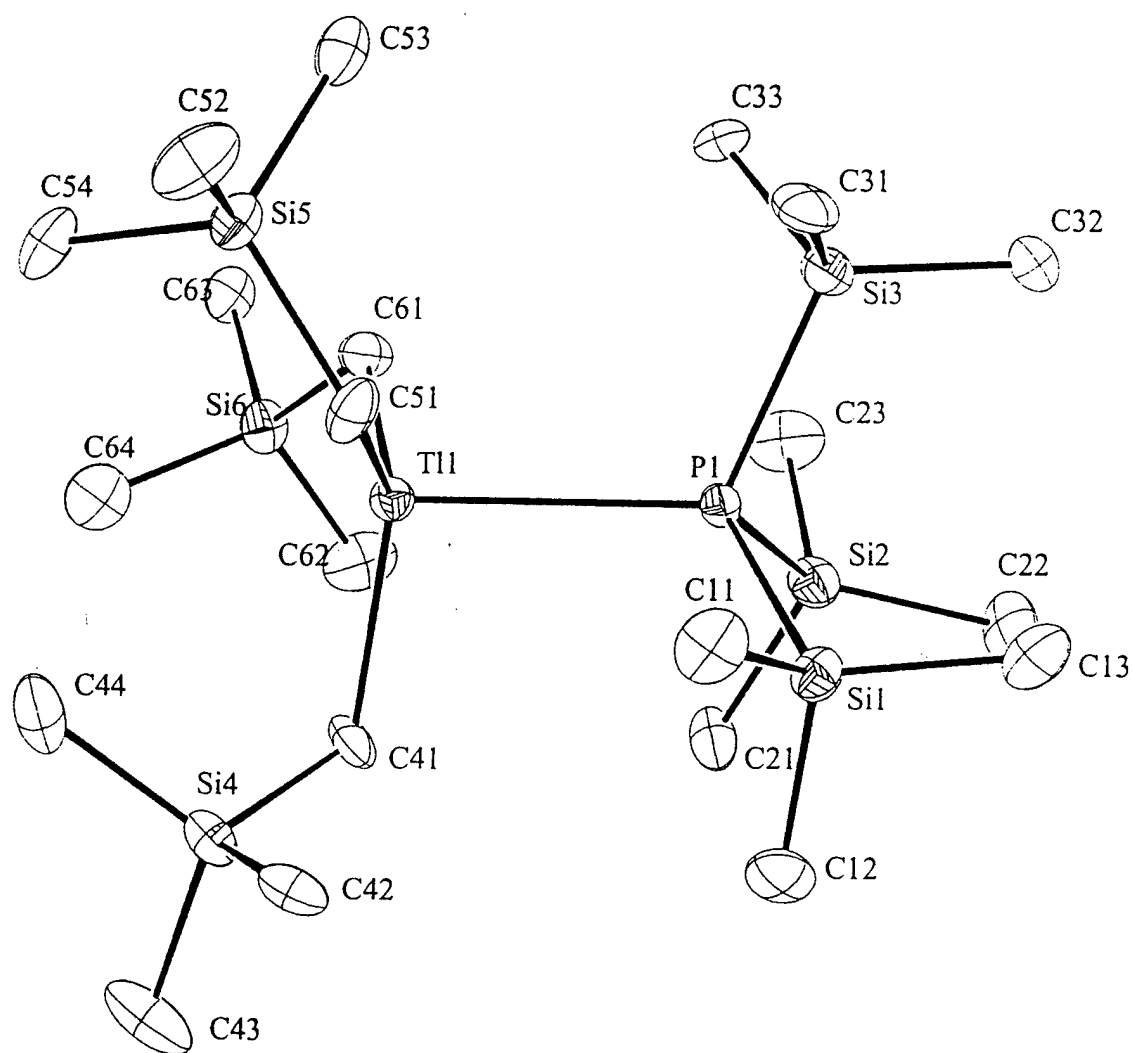
Additional material consisting of a summary of crystallographic data and measurements, atomic coordinates, thermal parameters, bond distances and angles, and structure factors (9 pages).

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Caption to Figure

Figure. ORTEP diagram (30% probability ellipsoids) showing the solid state structure and atom numbering scheme of **1**. Hydrogen atoms are omitted for clarity.



Figure

Table 1. Crystallographic Data and Measurements for $(\text{Me}_3\text{SiCH}_2)_3\text{Tl}\cdot\text{P}(\text{SiMe}_3)_3$ (1)

	1
molecular formula	$\text{C}_{21}\text{H}_{60}\text{PSi}_6\text{Tl}$
formula weight	716.55
crystal system	trigonal
space group	$\text{P}\bar{3}1$
a, Å	16.063(6)
c, Å	12.148(3)
V, Å ³	2714.3(11)
Z	3
radiation (wavelength, Å)	Mo-K α (0.71073)
μ , mm ⁻¹	4.75
temp, °C	-120
D _{calcd} , g cm ⁻³	1.315
crystal dims., mm	0.30 x 0.30 x 0.30
T _{max} ; T _{min}	0.360:0.300
scan type	ω
2 Θ _{max} , deg	50
no. of rflns recorded	3998
no. of non-equiv.	3998
rflns recorded	
no. of rflns retained,	3333
I > 2.5 σ (I)	

Table 1 (continued)

	1
no. of params.	262
refined	
R; R _w ^a	0.042; 0.045
goodness-of-fit ^b	1.21
max shift / esd. in final	0.012
least-squares cycle	
final max, min $\Delta\rho$, e/Å ⁻³	1.64; -1.24

$$^aR = \Sigma(|F_o| - |F_c|)/\Sigma|F_o| ; R_w = [\Sigma w_i (|F_o| - |F_c|)^2 / \Sigma w_i |F_o|^2]^{1/2}.$$

$$^b\text{Goodness-of-fit} = [\Sigma w_i \Delta^2 / (N_{\text{observations}} - N_{\text{parameters}})]^{1/2}.$$

Table 2. Bond Distances (Å) and bond angles (°) for **1**, with Estimated Standard Deviations in Parentheses

Bond Lengths			
Tl(1)-P(1)	2.922(3)	Si(3)-C(32)	1.87(2)
Tl(1)-C(41)	2.24(1)	Si(3)-C(33)	1.84(2)
Tl(1)-C(51)	2.23(2)	Si(4)-C(41)	1.85(2)
Tl(1)-C(61)	2.25(2)	Si(4)-C(42)	1.85(2)
P(1)-Si(1)	2.267(5)	Si(4)-C(43)	1.87(2)
P(1)-Si(2)	2.249(5)	Si(4)-C(44)	1.85(2)
P(1)-Si(3)	2.261(5)	Si(5)-C(51)	1.86(2)
Si(1)-C(11)	1.85(2)	Si(5)-C(52)	1.88(2)
Si(1)-C(12)	1.86(2)	Si(5)-C(53)	1.87(2)
Si(1)-C(13)	1.84(2)	Si(5)-C(54)	1.86(2)
Si(2)-C(21)	1.84(2)	Si(6)-C(61)	1.82(1)
Si(2)-C(22)	1.86(2)	Si(6)-C(62)	1.87(2)
Si(2)-C(23)	1.84(2)	Si(6)-C(63)	1.86(2)
Si(3)-C(31)	1.87(2)	Si(6)-C(64)	1.85(2)
Bond Angles			
P(1)-Tl(1)-C(41)	98.9(4)	P(1)-Si(3)-C(33)	107.7(5)
P(1)-Tl(1)-C(51)	95.1(4)	C(31)-Si(3)-C(32)	108.9(7)
P(1)-Tl(1)-C(61)	100.4(4)	C(31)-Si(3)-C(33)	109.4(7)
C(41)-Tl(1)-C(51)	116.5(5)	C(32)-Si(3)-C(33)	109.1(7)
C(41)-Tl(1)-C(61)	116.2(5)	C(41)-Si(4)-C(42)	109.3(7)
C(51)-Tl(1)-C(61)	121.1(5)	C(41)-Si(4)-C(43)	110.6(7)
Tl(1)-P(1)-Si(1)	110.7(2)	C(41)-Si(4)-C(44)	111.5(7)
Tl(1)-P(1)-Si(2)	113.7(2)	C(42)-Si(4)-C(43)	109.0(8)
Tl(1)-P(1)-Si(3)	113.1(2)	C(42)-Si(4)-C(44)	108.5(8)
Si(1)-P(1)-C(11)	105.8(2)	C(43)-Si(4)-C(44)	107.9(9)
Si(1)-P(1)-C(12)	107.1(2)	C(51)-Si(5)-C(52)	108.5(7)
Si(2)-P(1)-C(13)	105.9(2)	C(51)-Si(5)-C(53)	111.4(7)
P(1)-Si(1)-C(11)	109.9(5)	C(51)-Si(5)-C(54)	111.6(7)
P(1)-Si(1)-C(12)	108.7(5)	C(52)-Si(5)-C(53)	108.2(8)
P(1)-Si(1)-C(13)	114.2(5)	C(52)-Si(5)-C(54)	109.5(8)

Table 2, Continued.

C(11)-Si(1)-C(12)	109.5(8)	C(53)-Si(5)-C(54)	107.6(8)
C(11)-Si(1)-C(13)	107.3(8)	C(61)-Si(6)-C(62)	109.7(8)
C(12)-Si(1)-C(13)	107.1(8)	C(61)-Si(6)-C(63)	110.8(7)
P(1)-Si(2)-C(21)	108.1(5)	C(61)-Si(6)-C(64)	111.6(8)
P(1)-Si(2)-C(22)	112.9(6)	C(62)-Si(6)-C(63)	107.8(7)
P(1)-Si(2)-C(23)	107.9(5)	C(62)-Si(6)-C(64)	109.2(9)
C(21)-Si(2)-C(22)	109.5(8)	C(63)-Si(6)-C(64)	107.7(7)
C(21)-Si(2)-C(23)	109.0(8)	Tl(1)-C(41)-Si(4)	114.5(7)
C(22)-Si(2)-C(23)	109.3(9)	Tl(1)-C(51)-Si(5)	117.2(7)
P(1)-Si(3)-C(31)	108.1(5)	Tl(1)-C(61)-Si(6)	116.2(7)
P(1)-Si(3)-C(32)	113.5(5)		

Table 3. Non-Hydrogen Atom Fractional Coordinates and Equivalent Isotropic Thermal Parameters for **1**, with Estimated Standard Deviations in Parentheses

Atom	x	y	z	B _{iso} (Å ²) ^a
Tl	0.33779(7)	0.01648(3)	0.7786(-)	2.21(4)
P(1)	0.32523(23)	-0.01183(24)	1.0169(3)	2.11(17)
Si(1)	0.1976(3)	-0.1566(3)	1.0616(3)	2.76(20)
Si(2)	0.4544(3)	-0.0102(3)	1.0908(4)	2.97(23)
Si(3)	0.3082(3)	0.1011(3)	1.1091(3)	2.74(20)
Si(4)	0.2590(3)	-0.1886(3)	0.6235(4)	3.16(23)
Si(5)	0.1911(3)	0.1084(3)	0.6955(4)	2.85(20)
Si(6)	0.5662(3)	0.1635(3)	0.6747(4)	3.15(21)
C11	0.0902(10)	-0.1757(11)	0.9849(14)	3.8(8)
C12	0.2257(11)	-0.2520(10)	1.0249(14)	3.9(8)
C13	0.1666(12)	-0.1708(11)	1.2089(14)	4.3(9)
C21	0.4859(12)	-0.0840(13)	1.0033(13)	3.9(11)
C22	0.4335(13)	-0.0568(14)	1.2342(14)	5.0(12)
C23	0.5543(11)	0.1144(12)	1.0896(17)	5.0(11)
C31	0.1836(11)	0.0777(11)	1.0855(13)	3.5(8)
C32	0.3295(12)	0.1019(11)	1.2609(13)	3.7(9)
C33	0.3950(12)	0.2191(10)	1.0513(13)	3.3(9)
C41	0.3473(11)	-0.1126(11)	0.7290(12)	3.3(8)
C42	0.1394(11)	-0.2599(10)	0.6882(13)	3.7(9)
C43	0.2946(13)	-0.2726(15)	0.5602(17)	5.9(12)
C44	0.2450(12)	-0.1152(13)	0.5116(13)	4.8(10)
C51	0.1944(10)	0.0059(10)	0.7622(13)	3.4(7)
C52	0.0621(11)	0.0773(12)	0.6823(16)	4.9(10)
C53	0.2557(12)	0.2201(12)	0.7797(14)	4.0(9)
C54	0.2481(12)	0.1349(12)	0.5567(14)	4.4(10)
C61	0.4744(11)	0.1588(10)	0.7663(13)	3.6(8)

^aB_{iso} = the mean of the principal axes of the thermal ellipsoid

Table 3, Continued.

Atom	x	y	z	B _{iso} (Å ²) ^a
C62	0.6225(11)	0.0977(12)	0.7381(17)	5.1(11)
C63	0.6625(10)	0.2895(11)	0.6513(13)	3.7(8)
C64	0.5159(12)	0.1100(13)	0.5392(15)	4.8(10)

^aB_{iso} = the mean of the principal axes of the thermal ellipsoid

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